An accurate analytic solution to the Thomas-Fermi equation

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Abstract

The explicit analytic solution of the Thomas-Fermi equation thorough a new kind of analytic technique, namely the homotopy analysis method, was employed by Liao [?] (Appl. Math. Comp. 144, (2003)). However, the base functions and the auxiliary linear differential operator chosen were such that the convergence to the exact solution was fairly slow. New base functions and auxiliary linear operator to form a better homotopy are the main concern of the present paper. It is known that proper choice of base functions and auxiliary operator is extremely significant in gaining the exact solution in order to reduce the computational cost. The proposed homotopy here not only greatly reduces the computational efforts by at least doubling the convergence of the homotopy series, but also enlarges the convergence region of the homotopy series as compared with that of Liao [?]. Padé approximants to the obtained solutions increase the accuracy even to a higher degree. To support this, the explicit analytical expressions obtained using the proposed approach are compared with the numerically computed ones and those of Liao [?].

Key words: Analytic solution, Thomas-Fermi equation, Homotopy analysis method, Computational cost, Padé approximant

1. Introduction

Nonlinear phenomena are encountered in all areas of sciences and engineering. Even though the study of nonlinear equations is of great importance to many scientific researchers in various fields, it is very difficult to solve nonlinear problems and, in general, it is often more costly to get an analytic approximation than a numerical one to a given nonlinear problem [?].

Since the Thomas-Fermi equation is one typical not easy-to-find exact solution, the explorations of the solution have taken considerable attraction of many authors. The analytic approximations of the Thomas-Fermi equation were proposed by some different techniques such as the variational approach [?], the δ-expansion method [?, ?], the decomposition method [?, ?], see also [?, ?, ?]. Since the techniques used in these papers were mostly perturbative and limited, the solutions are obliged to be valid for certain regions with a decreasing accuracy.

In an aim to search for new and more effective analytical tools, Liao in 1992 [?, ?] proposed the homotopy analysis method which deforms a difficult nonlinear problem into easy linear counterparts. This is achieved by introducing an auxiliary parameter in the construction of an homotopy, which can provide a convenient way to control the convergence of the approximation series and adjust the convergence regions if necessary. A series of nonlinear problems were later attacked with the use of homotopy analysis method [?, ?, ?, ?, ?, ?] and [?, ?]. An elegant, simple and explicit analytic solution to the Thomas-Fermi equation was presented in [?]. One main drawback of the homotopy analysis method is that it's convergence to the exact solution becomes too time-consuming as the parameters involved in the equations are not treated rationally. This seems to be the reason why Liao in [?] was unable to obtain higher-order approximations for the solution of the Thomas-Fermi equation, but presented only the homotopy approximations with a percentage accuracy of at most first order. On the other hand, this order is inadequate to demonstrate convergence of the method to the true solution.

We in the present paper use homotopy analysis technique of Liao for the analytic calculation of Thomas-Fermi equation. Motivated by the study [?], we aim to show that the computational task during the implementation of the homotopy analysis method can be further reduced if the Thomas-Fermi equation is treated in a more rational manner. This is accomplished here by modifying the original approach of Liao [?]. Knowing that the choice of base functions and auxiliary linear differential operator is very important in the homotopy technique, see for example [?], new base functions and auxiliary linear differential operator are presented here. Unlike those of [?], using these new parameters it is shown here that the convergence of the homotopy can be greatly accelerated, even greater by the homotopy Padé approximants. In addition to this, the region of convergence is much improved with the present approach.

The following strategy is adopted in the rest of the paper. In §2. the basis of homotopy analysis method is laid out with an application to the nonlinear Thomas-Fermi equation. Analytic expressions for the solution are derived and compared with the numerical and previously published results in §3.. Finally conclusions follow in §4..

2. The Homotopy Analysis Method

The Homotopy analysis method was first proposed by the Chinese mathematician Liao [?]. This method is based on the homotopy and has several advantages. To underline, firstly its validity does not depend upon whether or not nonlinear equations under consideration contain small or large parameters, hence it can solve more of strongly nonlinear equations than the perturbation techniques. Secondly, it provides us with a great freedom to select proper auxiliary linear operators and initial guesses so that uniformly valid approximations can be obtained. Thirdly, it gives a family of approximations which are convergent in a larger region. Liao successfully applied the homotopy analysis method to solve some nonlinear problems in mechanics. For example, Liao in [?] gave a purely analytic solution of 2D Blasius's viscous flow over a semi-infinite flat plate, which is uniformly valid in the whole physical region.

The essential idea of this method is to introduce a homotopy parameter, say p, which varies from 0 to 1. At $p = 0$, the system of equations usually has been reduced to a simplified form which normally admits a rather simple solution. As p gradually increases continuously toward 1, the system goes through a sequence of deformations, and the solution at each stage is close to that at the previous stage of the deformation. Eventually at $p = 1$, the system takes the original form of the equation and the final stage of the deformation gives the desired solution. Here we apply it to solve the nonlinear Thomas-Fermi problem. Consider a differential equation used to calculate the electrostatic potential in the Thomas-Fermi atom model [?, ?], called the Thomas-Fermi equation with the boundary conditions

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} + \sqrt{\frac{u^3}{x}} = 0,\ u(x=0) = 1,\ u(x \to \infty) = 0, \tag{2.1}$$

which describes the spherically symmetric charge distribution about a many electron atom. Equation (2.1) is not amenable to exact treatment and, therefore, approximate techniques must be resorted to. There exists neither linear terms nor small or large parameters in equation (2.1), so the standard perturbation methods cannot be applied directly. Due to the fact that the homotopy analysis method requires neither a small parameter nor a linear term in a differential equation, one possibility to approximately solve equation (2.1) is by means of the homotopy analysis method.

We first rewrite the original equation (2.1) in the form

$$N(u) = xu''^2 - u^3 = 0; \quad u(0) = 1,\ u(\infty) = 0. \tag{2.2}$$

The essence to approximate a problem is to represent its solution by means of a complete set of base functions. Considering the boundary conditions in (2.2) and the physical meaning of u, Liao [?] chosen the set of base functions

$$\{(1 + x)^{-m} | m \geq 1\}. \tag{2.3}$$

As Liao [?] discusses in detail on the free falling problem, the selection of different sets of functions is possible all of which generate the same solution. Besides, the homotopy analysis method provides us with freedom to choose the initial guess and the auxiliary linear operator so that one can represent the solution of the Thomas-Fermi equation by distinct set of base functions. However, some set of base functions might cause a very slow convergence to the true solution. Therefore, if a proper choice is made while selecting a set of function a better convergence can be achieved which may save both time and resources while computing. Thus, we here take a different set of base functions from (2.3) in an aim to speed up the convergence to the exact solution and instead of (2.3) choose

$$\{\alpha(\alpha+\beta x)^{-\gamma m} | m \geq 1, \quad \alpha, \beta, \gamma \in R\} \tag{2.4}$$

to represent the solution $u(x)$ of (2.2) in the form

$$u(x) \;=\; \sum_{n=1}^{\infty} c_n \frac{\alpha}{(\alpha+\beta x)^{\gamma n}}, \tag{2.5}$$

where c_m's are coefficients. Notice that if we set $\alpha = \beta = \gamma = 1$ in (2.4-2.5), the base functions of Liao ([?]) in equation (2.3) are obtained. Therefore, our base functions are somewhat more general. The key to choose the parameters in (2.4) is that a better convergence rate can be captures as compared to the case of Liao [?]. It will be clear soon that some certain selections will indeed lead to high savings in the computational time of the approximate solution of Thomas-Fermi equation by accelerating its convergence.

Equation (2.4) provides us with the *rule of solution expression*. This rule is important in the frame of the homotopy analysis method. Considering the initial conditions in (2.2) and the *rule of solution expression* above described, it is obvious that

$$u_0(x) = \frac{\alpha}{(\alpha+\beta x)^{\gamma}} \tag{2.6}$$

is a good initial guess for $u(x)$ satisfying the boundary conditions in (2.2) exactly. We next choose here

$$L = \frac{\beta x + \alpha}{\alpha + \gamma} \frac{\partial^2}{\partial x^2} + \beta \frac{\partial}{\partial x}$$

as our auxiliary linear differential operator, which was found to be quite efficient for the consideration of the present nonlinear problem, which has the property that $L(C_1(\alpha+\beta x)^{-\gamma} + C_2) = 0$, with C_1 and C_2 arbitrary constants. We are now at the stage of constructing the zeroth order deformation equation system associated with the Thomas-Fermi problem given by (2.2), which is also called a family of differential equations (viewing p as a parameter)

$$(1-p)L(u) \;=\; phN(u), \quad u(0,p) - 1 = u(\infty, p) = 0. \tag{2.7}$$

It should be noted that the nonlinear differential operator in equation (2.5) is given as in (2.2). Moreover, the parameter h is an auxiliary non-zero parameter to adjust the convergence rate of the perturbation series, which was found to be $-1/2 \leq h < 0$ in [?] for the convergence. However, in our case we will show that the region of h for the convergence can be extended. Obviously when $p = 0$ and $p = 1$, we have respectively

$$u(x, 0) = u_0(x), \quad u(x, 1) = u(x). \tag{2.8}$$

Hence the process of giving an increment to p from 0 to 1 is the process of $u(x, p)$ varying continuously from the initial guess $u_0(x)$ to the final solution $u(x)$. This kind of continuous variation is called deformation in topology so that we call system (2.7) the zeroth order deformation equation. Next, differentiating (2.7) successively and eventually imposing at $p = 0$, the kth-order deformation equations follow as

$$L(u_k) = L(u_{k-1}) + hR_k, \quad u_k(0) = u_k(\infty) = 0. \tag{2.9}$$

The function R_k on the right-hand side of (2.9) is given by

$$R_k = \frac{1}{(k-1)!} \frac{\partial^{k-1} N}{\partial p^{k-1}}|_{p=0}.$$

Finally, a straightforward Taylor expansion of $u(x, p)$ at the point $p = 0$ and eventually imposing the series at $p = 1$ gives the solution of system (2.2) in the form

$$u(x) = u_0(x) + \sum_{k=1}^{\infty} u_k(x), \tag{2.10}$$

for which we presume that the initial guesses u_0 to u, the auxiliary linear operator L and the non-zero auxiliary parameter h are all so properly selected that the deformations $u(x, p)$ are smooth enough and their kth-order derivatives with respect to p in equation (2.9) exist and are given by $u_k = \frac{1}{k!}\frac{\partial u}{\partial p}|_{p=0}$. It is clear that the convergence of Taylor series at $p = 1$ is a prior assumption here so that the system in (2.10) holds true. The formulae in (2.10) provide us with a direct relationship between the initial guesses and the exact solutions. Moreover, a special emphasize should be placed here that the kth-order deformation system (2.9) is a linear differential equation system with the auxiliary linear operator L whose fundamental solution is known as aforementioned. Eventually, we obtain the result at the Nth-order approximation as

$$u(x) = \sum_{k=0}^{N} u_k(x). \tag{2.11}$$

3. Results and discussion

In this section analytic approximate solutions corresponding to system (2.2) is presented. Solutions obtained from the homotopy analysis method are compared with those obtained from the full numerical computations and the available solution of [?].

Note that the analytic solution presented in (2.11) contains the auxiliary parameter h, which can be employed to control the convergence of approximations and adjust convergence regions when necessary. As claimed before, the proper choice of parameter α, β, γ can yield an extended convergence region as compared to the case of Liao [?].

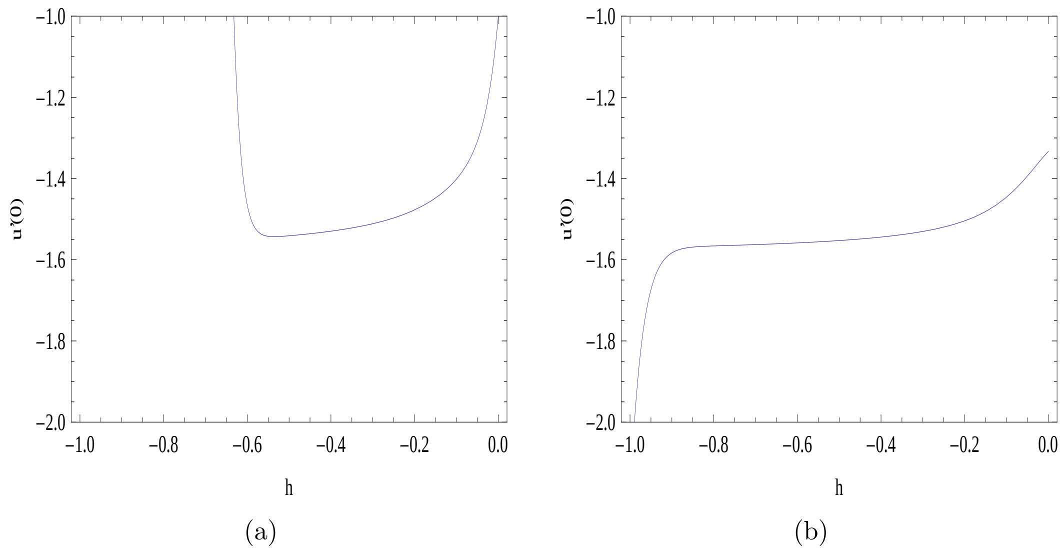

Figure 1: The $h-$ curves of $u'(0)$ obtained from the 20th-order homotopy approximation solution of the problem (2.2). (a) Case of Liao [?] ($\alpha = \beta = \gamma = 1$), (b) the present case ($\alpha = 3/4, \beta = \gamma = 1$).

To illustrate this, the influence of h on the convergence of the solution series are given in figures 1(a-b). The $h-$curves are drawn for $u'(0)$ obtained from the 20th-order homotopy analysis approximation. Figure 1(a) depicts the case of [?] (not given in [?]) and 1(b) depicts our case. As found by Liao in [?], when h is restricted to $-1/2 \leq h < 0$, the series in (2.11) converges in the whole region $0 \leq x < \infty$, which is indeed the case as shown in figure 1(a). On the other hand, for the parameters $\alpha = 3/4$, $\beta = \gamma = 1$, we are able to extend the convergence region of h to $-9/10 \leq h < 0$, as shown in figure 1(b). This is important since in a larger region of convergence a better convergence rate can be achieved for the series. In fact, it is easy to see that in order to have a good approximation

h has to be chosen around $-4/5$. When $h = -4/5$, the analytic result at the

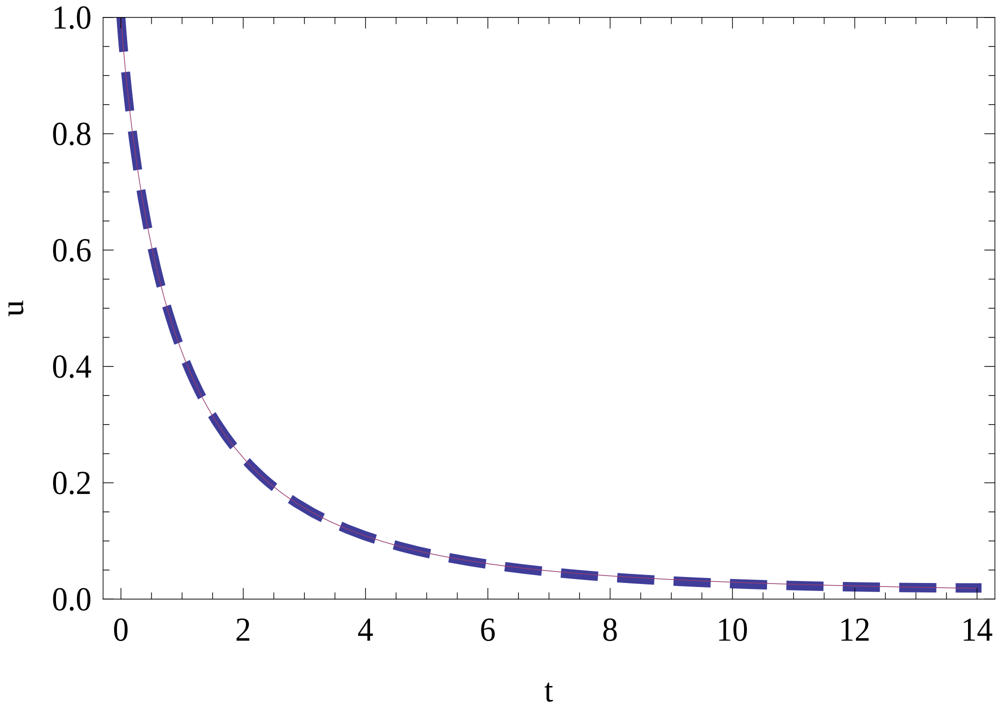

Figure 2: Comparison of the analytic result of the Thomas-Fermi equation with the numerical result. Solid line denotes analytic result at the 40th-order approximation for $h = -4/5$ and dashes denote the numerical result.

40th-order of approximation agrees well with the numerical result, as shown in figure 2. As compared with the 60th-order of approximation of Liao [?] (see figure 2 of Liao [?]) our analytic solution at a lower order is clearly seen to better approach the exact solution. To explain the reason deeply, and in fact to disclose the difference between our solution and that of Liao [?], we list in table 1 the values of initial slope $u'(0)$ (which is used to obtain the energy of a neutral atom in the ThomasFermi model, see [?]) and curvature $u''(0)$ respectively. The error between the exact and approximate $u'(0)$ is also given in table 1. Obviously, the error decreases as the order of approximation increases, in both our case and the case of Liao [?]. However, more importantly, the convergence of our series (2.11) is seen to be more than twice as the convergence of the iterations of Liao [?]. This justifies the claim that our base functions indeed approximate the exact solution of Thomas-Fermi equation at a better convergence rate. This as a result will save us both in terms of computational time and resources. Moreover, owing to equation (2.2), it holds $u''(0) \to \infty$ as $x \to 0^+$. The approximations of $u''(0)$ obtained from the homotopy analysis method when $h = -3/4$ are listed in table 1 show

that $u''(0)$ of the analytic solution (2.2) indeed tends to infinity. Again, the trend is observed to be twice as high as the trend of Liao [?]. The remarkable accuracy of the results tabulated clearly illustrate the effectiveness and efficiency of the proposed approach. Table further reveals as claimed before that the presented approximate solutions take less computational time as compared with that of [?].

N	$u'(0)$	Error(%)	$u'(0)^L$	$u''(0)$	$u''(0)^L$
10	-1.54628	2.63	-1.50014	25.4567	13.0003
20	-1.56597	1.39	-1.54093	46.8426	23.0819
30	-1.57305	0.94	-1.55595	68.1948	33.1119
40	-1.57669	0.71	-1.56373	89.5378	43.1275
50	-1.57891	0.57	-1.56848	110.877	53.1370
60	-1.58040	0.48	-1.57168	132.214	63.1434
70	-1.58171	0.40	-1.57399	151.216	73.1480
80	-1.58303	0.31	-1.57572	173.012	83.1514
90	-1.58424	0.24	-1.57708	196.871	93.1542
100	-1.58515	0.18	-1.57816	224.112	103.1560

Table 1: Analytic approximations of $u'(0)$ and $u''(0)$ when $h = -3/4$, the percentage error occurred for $u'(0)$ and comparison of the results with those of Liao [?], denoted by a superscript L.

As implemented in [?], we can further employ the [m,m] diagonal homotopy Padé approximants [?] to the power series of $u'(0)$ in order to gain more accurate approximations of the initial slope, as shown in table 2. Note that the error decreases with the increase of the degree of the Padé approximants. Comparisons with the Padé approximations of Liao [?] once more shows the better accuracy obtained from the present approach.

Padé approximants	$u'(0)$	Error(%)	$u'(0)^L$
$[10, 10]$	-1.58030	0.48933	-1.51508
$[20, 20]$	-1.58571	0.14867	-1.58281
$[30, 30]$	-1.58694	0.07122	-1.58606
$[40, 40]$	-1.58752	0.03469	-1.58668
$[50, 50]$	-1.58801	0.00384	-1.58712

Table 2: Approximations of the initial slope $u'(0)$ given by the diagonal Padé approximants, when $h = -3/4$ and the percentage error occurred. Comparisons with $u'(0)$ obtained by Liao [?] is denoted by the superscript L.

4. Concluding remarks

In this paper, the homotopy analysis method has been applied to obtain approximate analytical solution for nonlinear phenomena governed by the Thomas-Fermi equation. The results presented have readily revealed that the approach adopted is very effective and convenient. Comparisons of the approximations with the published ones of Liao [?] have proven the accuracy and efficiency of the proposed approach which rapidly doubles the convergence rate of the homotopy series solution to the exact solution and hence significantly reduces the time consumption while evaluating the approximate analytic solutions thorough the homotopy analysis method.

The key to get fast convergence and better accuracy as compared with that of Liao [?] has been to select more appropriate different set of base functions and auxiliary linear differential operator. Such a rational choice has been shown to enlarge the region of convergence of the homotopy series and thus yield acceleration of the convergence. Diagonal homotopy Padé approximants to the power series obtained have been shown to improve some degree the accuracy and convergence of the homotopy series to the exact ones.

The purely explicit analytical solutions obtained here also provide a good scientific base for the validation of the numerically computed values using different schemes in the literature. In addition to this, the developed approach could be expected to be applicable to attain the solutions of highly nonlinear systems arising from the applications in engineering and science.